Fast, High-Order, High-Frequency "Accurate Fourier Methods" for Scattering Problems

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Introduction. We present a new set of algorithms and methodologies for the numerical solution of problems of scattering by complex bodies in three-dimensional space. These methods, which are based on integral equations, high-order integration, fast Fourier transforms and highly accurate high-frequency methods, can be used in the solution of problems of electromagnetic and acoustic scattering by surfaces and penetrable scatterers — even in cases in which the scatterers contain geometric singularities such as corners and edges. In all cases the solvers exhibit high-order convergence, they run on low memories and reduced operation counts, and they result in solutions with a high degree of accuracy.

Theoretical Background. Many aspects of our methods resulted from consideration of the remarkable properties exhibited by the trapezoidal rule for integration of smooth periodic funtions over d-dimensional cubes ($d = 1, 2, \ldots$). Of course the integrals arising in integral equation formulations involve surfaces which are much more complex that a square in 2-dimensions or a cube in 3-dimensions, and they require consideration of highly non-smooth integrands — which arise from both, singularities in the Green functions and from the geometric sigularities of the scatterer: edges, corners, etc. As we have shown, however, appropriate transformations permit one to obtain high-order integrators from trapezoidal rules and Fourier series. Further, use of fast Fourier transforms for evaluation of Fourier series and convolutions allows for fast numerics in addition to high accuracy. To demonstrate these facts in simple settings we preface our discussion by a number of considerations on the properties of the trapezoidal rule and Fourier series for functions under various periodicity and smoothness assumptions.

Let us thus consider the basic problem of integration of a function $y = f(x)$ over a one-dimensional interval $[a, b]$. Table 1 displays relative errors and convergence ratios for three problems which encapsulate some of the relevant issues under consideration: $\int_0^{1/2} \sqrt{x}dx$; $\int_0^{\pi/4} e^{cos^2(x)}dx$ and $\int_0^{\pi} e^{cos^2(x)}dx$. From Table 1 we see that integration of the non-smooth function $\sqrt{x}$ results in errors of the order $\mathcal{O}(h)$ for a grid of mesh-size h: refinement of the mesh by a factor of 2 leads to error reductions by the same factor. When applied to integration of the smooth function $f(x) = e^{cos^2(x)}$ over the interval $[0, \pi/4]$, in turn, the trapezoidal rule results in quadratic errors: refinement of the mesh by a factor of 2 leads to error reductions by a factor of 4. In the last case in which the *smooth and periodic* function $f(x) = e^{cos^2(x)}$ is integrated over its peridod, we see a enormously higher, exponential convergence rate.

The behavior exhibited by the trapezoidal rule is easy to explain. As is well known, for a general smooth function, the trapezoidal rule gives rise to quadratic errors, as shown in Table 1 center, since the error in the approximation of an integration element of mesh-size h by its trapezoidal approximation is of the order of h^3. For non-smooth functions that basic-element error goes down to h^2, and it results in overall errors which are linear on h. A phenomenon of a different nature takes place as integration of smooth and periodic functions is considered. The reason for this extraordinary phenomenon is different from those arising in the previous two cases. The operative elements in this case are 1) The extremely fast convergence of Fourier series of smooth periodic functions, and, 2) The

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N	Rel. Error	Ratio
1	4.69(-1)	
2	2.04(-1)	2.30
4	8.99(-2)	2.27
8	4.02(-2)	2.24
8192	2.72(-5)	

N	Rel. Error	Ratio
1	4.77(-2)	
2	1.19(-2)	4.03
4	2.95(-3)	4.02
8	7.36(-4)	4.01
8192	7.01(-10)	

N	Rel. Error	Ratio
1	5.50(-1)	
2	6.03(-2)	9.12
4	3.10(-4)	1.95(2)
8	7.17(-10)	4.32(5)
16	2.10(-23)	3.42(13)

Table 1: Relative errors in trapezoidal-rule approximations for $\int_a^b f(x)dx$ using N intervals ($N+1$ discretization points). Left: $f(x) = \sqrt{x}$, $a = 0$, $b = 1/2$. Center: $f(x) = e^{cos^2(x)}$, $a = 0$, $b = \pi/4$. Right: $f(x) = e^{cos^2(x)}$, $a = 0$, $b = \pi$.

remarkable fact that the trapezoidal rule $N+1$ points (N intervals) integrates exactly the Fourier harmonics $e^{i\ell x}$ for $\ell = -N \ldots N$. From Table 1 we thus see that use of 8 integration intervals for integration of the smooth periodic function $f(x) = e^{cos^2(x)}$ in its periodicity interval results in errors of the order of 10^{-10}. For the non-periodic integration problem in Table 1 center, an equivalent accuracy requires 8192 intervals. And, use of this highly refined mesh gives an accuracy of only 10^{-5} when the integration problem for the non-smooth function $\sqrt{x}$ is considered.

With regards to engineering relevance of the accuracy exhibited by high order numerical methods, it has been correctly argued that seldom an accuracy better than 1%-0.1% is significant in engineering problems arising in practice. While this is true in many cases, it is our contention that high-order accuracy is nevertheless essential in applications. Indeed, the fast convergence arising from high-order methods allows for an understanding of the errors incurred in a given calculation. Certainly, estimation of the accuracy of a certain approximation requires, say, the possibility of evaluation of the solution to at least one additional digit of accuracy. With first order convergence (which, as demonstrated clearly by Table 1, necessarily results from a simple-minded integration method) requires a refinement of the mesh by a factor of ten. For the two-dimensional integrals we are considering this translates into a factor of $10^2 = 100$ in the number of discretization points — and thus, in the number of unknowns in the problem! Clearly, refinement of a first order algorithm is not a viable approach for evaluation of the accuracy of a numerical solution. A high-order algorithm such as that used in Table 1 right, in turn, can give us an additional digit of accuracy (and, therefore, a good measure of the accuracy of a numerical solution) by an increase of a few percent in the overall size of the numerical problem. This is an extremely valuable feature in a numerical method which, as mentioned above, we seek through consideration of the trapezoidal rule for smooth functions, and the high order convergence of Fourier series for smooth periodic functions. Fast numerics in our setup, in turn, result from use of $\mathcal{O}(N \log(N)$ fast Fourier transforms.

As discussed above, the functions naturally arising in integral equation approaches for three-dimensional problems are neither smooth nor periodic — thus our efforts which have reduced general integration problems of a non-smooth function in an arbitrary domain to a sequence of one-dimensional integration problems for smooth functions. Some elements in our methods include

1. **Partitions of unity** [5]: We use a covering of the surface or volume by a number K of overlapping patches $\mathcal{P}^j, j = 1, \cdots, K$, (called local charts in differential geometry). The patches $\mathcal{P}^j$ are then smoothly mapped to cartesian sets $\mathcal{H}^j$, where actual integrations are performed. Further, we utilize a partitions of unity subordinated to these coverings of the integration domain, i.e. we introduce a set of non-negative smooth functions $\{w^j, j = 1, \ldots, K\}$, such that (i) w^j is defined, smooth and non-negative in integration domain, and it vanishes outside $\mathcal{P}^j$, and (ii) $\sum_{j=1}^K w^j = 1$ throughout the integration domain. This allows us to reduce the

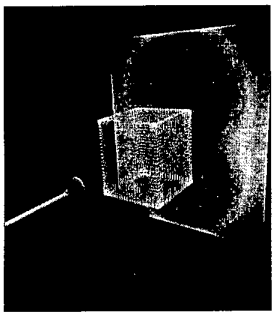

Figure 1: Scattering by a perfectly conducting cube; electric field polarized horizontally.

problem of integration of the density $\varphi(\mathbf{r})$ over the surface/volume to a calculation of integrals of smooth functions φ^j compactly supported in the planar sets $\mathcal{H}^j$ multiplied by the singular Green's function.

2. **Adjacent integration** [1, 2, 5]: While, certainly, the well-known strategy of "singularity subtraction" gives rise to bounded integrands, integration of such bounded functions by means of classical high-order methods does not exhibit high-order accuracy — since the subsequent derivatives of the integrand are themselves unbounded. The new basic high-order integrators we use are based on analytical resolution of singularities. The resolution is achieved by integration in polar coordinates centered around each singular point. The Jacobian of the corresponding changes of variables has the effect of cancelling the singularity, so that high order integration in the both radial and angular directions can be performed using the trapezoidal rule.

3. **Acceleration** [5]: Our accelerator is closely related to two of the most advanced FFT methods developed recently [9, 14]. An important common element between these two methods and our technique is a concept of equivalent (or auxiliary) sources, located on a subset of a 3-D Cartesian grid. In all three cases, the intensities of these sources are chosen to approximate the field radiated by the scatterer, which allows for fast computation of the "non-adjacent interactions" through the use of 3-D FFTs. Surface problems like the ones we consider are treated in [9, 14] by means of equivalent sources located in a *volumetric* grid — in such a way that equivalent sources with non-zero intensities occupy *all Cartesian nodes adjacent to the scatterer.* Since the spacing of this Cartesian grid cannot be coarsened beyond some threshold for surface problems such a scheme requires a $\mathcal{O}(N^{3/2})$ FFT. Therefore, previous FFT surface scattering solvers require $\mathcal{O}(N^{3/2})$ units of RAM and they run in $\mathcal{O}\left(N^{3/2}\log N\right)$ operations. Our algorithm, in contrast, subdivides the volume occupied by the scatterer into a number of (relatively large) cubic cells, and it places equivalent sources *on the faces* of those cells. As we have shown, such a design reduces significantly the sizes of the required FFTs — to as little as $\mathcal{O}\left(N^{6/5}\right)$ to $\mathcal{O}\left(N^{4/3}\right)$ points — with proportional improvement in storage requirements and operation count. Further, it results in super-algebraic convergence of the equivalent source approximations *as the size of the scatterer is increased.*

Numerical Results. In this section we describe the results of our solvers in a number of additional scattering geometries, and we present specific results for a well known scatterer, the

electromagnetic cube. In previous work we have successfully tackled some of the largest benchmark problems ever considered. In particular we obtained solutions for an acoustic ellipsoid with $(ka, kb, kc) = (100, 25, 25)$ with far-field errors of the order of 10^{-4} [5]. These computations were performed in a 400MHz Pentium II PC; competing calculation for this scatterer, with no accuracy estimates given, were performed in supercomputing infrasctructures. Computations for large spheres, in turn, have resulted in accuracy improvements of the order of several orders of magnitude over other methods, with computing times in 400MHz Pentium II computers which are lower than those used by other methods in high-performance computers. The specific results for the EM cube depicted in Figure 1, finally, concern a highly singular geometry with $ka = 3.3$ for which errors are of the order of 10^{-5}. Details on the singularity resolution strategies for the cube edges are given in [8]. We see that high-order accuracy in fast computing time can be achieved by these methods even for highly singular electromagnetic scatterers.

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